



chain nodes :

13 14 17 18 20 21 23 27 28

ring nodes :

1 2 3 4 5 6 7 8 9 10 11 12

ring/chain nodes :

24

chain bonds :

2-23 4-17 5-13 6-18 7-21 9-14 11-20 12-27 13-14 23-24 27-28

ring bonds :

1-2 1-6 2-3 3-4 4-5 5-6 7-8 7-12 8-9 9-10 10-11 11-12

exact/norm bonds :

2-23 4-17 6-18 7-21 11-20 12-27 23-24

exact bonds :

5-13 9-14 13-14 27-28

normalized bonds :

1-2 1-6 2-3 3-4 4-5 5-6 7-8 7-12 8-9 9-10 10-11 11-12

G1:C,O

G2:H,F

G3:CN,CF3,N

Match level :

1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:Atom 8:Atom 9:Atom 10:Atom 11:Atom  
 12:Atom 13:CLASS 14:CLASS 17:CLASS 18:CLASS 20:CLASS 21:CLASS 23:CLASS 24:CLASS  
 27:CLASS 28:CLASS